9–4 Prevention of Hydrogen Embrittlement in Aluminum Alloys

— Identification of the Intermetallic Compounds that Take Away Hydrogen from Aluminum Lattice —

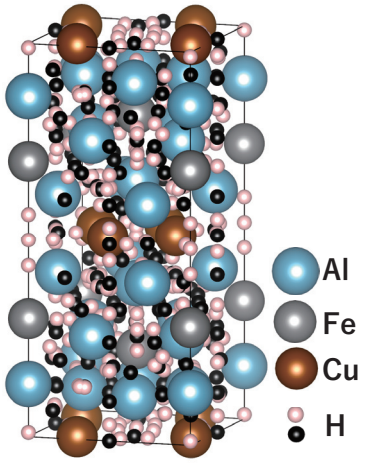

Fig.9-7 Crystal structure of an Al_7FeCu_2 compound and position of hydrogen atoms
Hydrogen (H) atoms can take two positions: the light-colored sphere lies at the vertex of the Voronoi polyhedron centered on the lattice points of Al, Fe, and Cu atoms, and the black sphere lies at the center of the plane of the polyhedron.

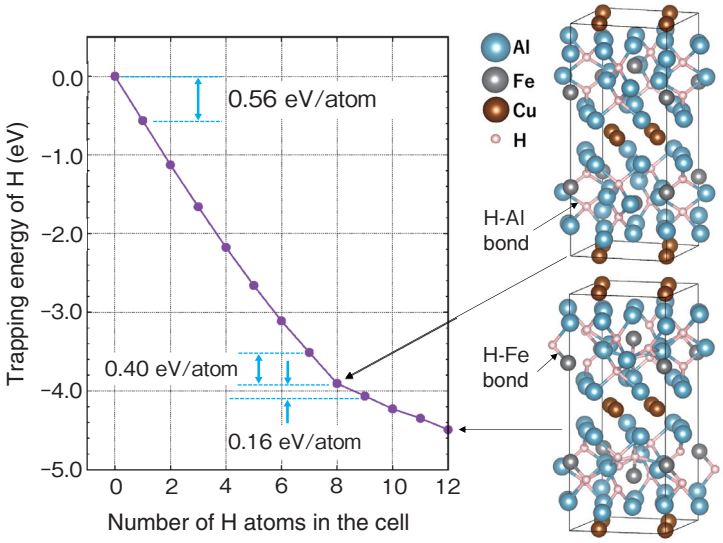

Fig.9-8 Hydrogen storage capacity of Al_7FeCu_2 compounds in aluminum
Initially, absorbed H atoms have a considerable trapping energy of 0.56 eV/atom in the cell. Because this decreases with the number of H atoms absorbed, approximately eight hydrogen atoms are expected to be absorbed in a cell of forty Al, Fe, and Cu atoms.

Although aluminum alloys have been commercially used for decades, significant improvements to their strength have not been made in many years. It has long been known that the strength of aluminum alloys, such as duralumin, which is used in aircraft bodies, has been improved by adding more zinc elements several ten years ago. However, adding alloying elements in this fashion tends to produce high-strength aluminum alloys that are susceptible to fracture due to hydrogen embrittlement because hydrogen penetrates the material during manufacturing. Hydrogen is the smallest element and thus can move quickly inside an aluminum lattice. Further, clarifying the behavior of hydrogen inside a lattice is difficult; the impact of hydrogen on the deformation and fracturing of an alloy has not been characterized well. However, reducing the hydrogen concentration in an aluminum alloy could prevent hydrogen embrittlement.

Thus, a compound that absorbs hydrogen in aluminum alloys and increases its concentration could prevent hydrogen embrittlement of aluminum lattice, because it reduces the content of hydrogen in aluminum lattice. Using first-principles calculations to investigate various compounds' ability to absorb hydrogen, we discovered that an Al_7FeCu_2 compound strongly absorbs hydrogen.

The crystal structure of the Al_7FeCu_2 compound and the possible interstitial sites where hydrogen atoms can be absorbed are shown in Fig.9-7. Here, a Voronoi polyhedron division method was used to find the positions where hydrogen atoms are likely to enter. Next, the positions that could trap hydrogen atoms firmly were found by calculating the trapping energy from first-principles calculations. Furthermore, as shown in Fig.9-8, the amount of hydrogen absorbed in the cell was calculated.

Experimental work confirmed the effect of suppressing hydrogen embrittlement by increasing the Al_7FeCu_2 content in an aluminum alloy. Therefore, we submitted a patent application in Japan with Kyushu University detailing this embrittlement prevention method and alloy that is less susceptible to hydrogen embrittlement (Japanese Patent Application No.2020-96333).

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Reference

Yamaguchi, M. et al., Hydrogen Trapping in Mg_2Si and Al_7FeCu_2 Intermetallic Compounds in Aluminum Alloy: First-Principles Calculations, Materials Transactions, vol.61, issue 10, 2020, p.1907–1911.